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TITLE ELASTIC NEUTRON SCATTERING IN UCd_{11}

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Abstract

We report results of neutron powder diffraction experiments on the heavy-electron magnet UCd_{11} at temperatures above and below its ordering temperature. These measurements set an upper limit on the ordered moment of $1.5\mu_B$/U.

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Specific heat measurements on UCd_{11} show a large electronic contribution ($\gamma \simeq 840$ mJ/mole K^2) above 5K, at which temperature occurs an anomaly indicative of a magnetic phase transition in the bulk [1]. Associated with this anomaly is a very weak feature in the magnetic susceptibility. More recent muon-spin rotation/relaxation measurements [2] suggest antiferromagnetic order at 5K but neither the ordered moment nor magnetic structure could be determined from these experiments. For the two other U-based heavy-electron magnets U_2Zn_{17} [3] and UCu_5 [4], neutron scattering experiments have established that the magnetic order is simple antiferromagnetic, with ordered moments of 0.8 ± 0.1 and 0.9 ± 0.1 μ_B/U respectively, values close to 1/3 of their corresponding paramagnetic moments. Interestingly, the factor 1/3 also appears in the ratio of their electronic specific heat γ below T_N to that above T_N [5]. UCd_{11} also exhibits the ratio $\gamma(T = 0)/\gamma(T \gtrsim T_N) = 0.3$ [1] from which, if the analogy holds, we would imply an ordered moment of $\gtrsim 1$ μ_B/U.

To minimize the problem associated with the extremely large neutron absorption cross-section of naturally abundant Cd, we have performed neutron diffraction on samples enriched to 98.55% Cd^{114}, which has a much smaller absorption cross section. An approximately 5 g sample was prepared by sealing under vacuum fine U powder in a quartz tube with distilled Cd^{114} and heating to 470°C for 7 days. X-ray analysis of the reacted powder showed the material to be $\gtrsim$ 97% UCd_{11}, having the Pm3m crystal structure with a lattice parameter $a_0 = 9.290$ Å. Magnetic susceptibility measured on 85 mg of the sample showed Curie-Weiss behavior for 20 < T < 350K, with $\mu_{eff} = 3.86$ μ_B/U and $\theta = -46.6$ K, and a plateau near 5 K, characteristic of the magnetic transition in UCd_{11}.

Neutron scattering was performed on the General Purpose Powder Diffractometer at Argonne's Intense Pulsed Neutron Source. For these experiments, the 5 g sample was encapsulated in a thin-walled aluminum holder that was mounted on the cold finger of a ^{4}He cryostat whose temperature could be controlled down to 2K. Parts of the sample holder exposed to the neutron beam and not containing sample were masked by a boron-nitride shield. Approximately 20 hours of data were collected at three temperatures 8, 4, and 2K. Each data set was analyzed by Rietveld refinement using the codes developed by Larson and Von Dreele [6].

Results of the measurements at 2K are shown in Fig. 1. In fitting these data, it was necessary to include scattering from the Al sample holder, BN mask, and "displaced" Al arising from scattering off the Al tail of the cryostat. In addition, to the majority phase UCd_{11}, we also found evidence for a small amount (~ 2%) of free Cd, in agreement with the x-ray analysis. By taking these scattering sources into account, all peaks (except one with d = 1.409 $\mathring{A}$) could be indexed and the refined parameters for UCd_{11} are given in Table I. The unidentified peak also appeared in the 4 and 8K spectra. Additional structural details of UCd_{11} will be given elsewhere [7] but we note here that assuming unity occupation of the U-site gives a stoichiometry of $UCd_{9.5}$ and that no structural change could be detected to within $\Delta a_0 = \pm 0.00008$ $\mathring{A}$. Further, within the resolution of these experiments, no additional lines could be found below 5K that might be expected to appear because of antiferromagnetic order.

A minimum detectable moment was estimated assuming a simple ferromagnetic structure, which would provide an upper limit. We assume that a magnetic peak would be observed if its intensity were greater than the (3,0,0)/(2,1,1) nuclear peak indicated by the arrow in Fig. 1(c).

Because the structure factor of this peak is known, we can calculate a limit of detectability to be 1.5 μ_B/U. Therefore, we conclude that the ordered moment of "UCd_{11}" must be less than 1.5 μ_B/U, that the magnetic structure is not simple, or possibly both. The first conclusion is implicated on the basis of analogy to other U-based heavy-electron magnets.

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TABLE I

Crystal Data for UCd_{11} at 2 K

Space Group Pm3m $\quad a_0 = 9.2480(8)$ Å

Atomic Positions

Atom	x	y	z	u(Å^2)	Fraction
U1	0	1/2	0	0.0072(5)	1
Cd1	1/2	1/2	1/2	0.0033(13)	0.81(3)
Cd2	0.1567(2)	0.1567(2)	0.1567(2)	0.0063(6)	0.94(1)
Cd3	0	0.3441(2)	0.3441(2)	0.0082(5)	0.87(1)
Cd4	1/2	0.2664(1)	0.2664(1)	0.0078(4)	0.88(1)

Figure Caption

Fig. 1. Time-of-flight neutron diffraction spectra for UCd_{11} at 2K. Data in panels (a) and (b) were collected with detectors at $2\theta = 148°$ and those in (c) with $2\theta = 90°$. Crosses are data, the solid line is the Rietveld fit and the lower curve in (a) and (b) is the residual. Vertical tick marks indicate d-spacings of Bragg reflections for UCd_{11}, Al, Cd, BN, and displaced Al, respectively, from the bottom set upwards.

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